Strongly Anisotropic $S = 1$ (Pseudo) Spin Systems: from Mean Field to Quantum Monte-Carlo

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The $S = 1$ pseudospin formalism was recently proposed to describe the charge degree of freedom in a model high-$T_c$ cuprate with the on-site Hilbert space reduced to the three effective valence centers, nominally Cu$^{1+ ; 2+ ; 3+}$. With small corrections the model becomes equivalent to a strongly anisotropic $S = 1$ quantum magnet in an external magnetic field. We have applied a generalized mean-field approach and quantum Monte-Carlo technique for the model $2D \ S = 1$ system to find the ground state phase with its evolution under deviation from half-filling and different correlation functions. Special attention is given to the role played by the on-site correlation (“single-ion anisotropy”).

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1. Introduction

These days spin algebra and spin Hamiltonians are used not only in the traditional fields of spin magnetism but in so-called pseudospin lattice systems with the on-site occupation constraint. For instance, the $S = 1$ pseudospin formalism was applied to study an extended Bose-Hubbard model (EHBHM) with truncation of the on-site Hilbert space to the three lowest occupation states $n = 0, 1, 2$ (semi-hard-core bosons) considered to be three pseudospin states with $M_S = -1, M_S = 0, M_S = +1$, respectively (see Ref. [1] and references therein). At variance with quantum $s = 1/2$ systems the Hamiltonian of $S = 1$ spin lattices in general is characterized by several additional terms such as a single ion anisotropy that results in their rich phase diagrams. Recently we made use of the $S = 1$ pseudospin formalism to describe the charge degree of freedom in high-$T_c$ cuprates with the on-site Hilbert space reduced to only the three effective valence centers [CuO$_4$]$^{7- ; 6- ; 5-}$ (nominally Cu$^{1+ ; 2+ ; 3+}$) [2–5].

2. $S = 1$ (pseudo) spin Hamiltonian

The $S = 1$ spin algebra includes the eight nontrivial independent spin operators: spin-dipole moment $S$ and five spin-quadrupole operators $Q_{ij} = (\hat{i}/2 [S_i, S_j] - \hat{j} \delta_{ij})$ whose mean values define so-called spin-nematic order. Spin operators $S_{\pm}$ and $T_{\pm} = [S_x, S_{\pm}]$ change the pseudospin projection (and occupation number!) by $\pm 1$, while $S_{\pm}$ changes the pseudospin projection by $\pm 2$.

Hereafter in the paper we will focus on a simplified $2D \ S = 1$ (pseudo) spin Hamiltonian with the nearest neighbor coupling and the only two-particle transport term (inter-site biquadratic anisotropy) as follows:

$$\hat{H} = -t \sum_{\langle ij \rangle} (S_{i+}^2 S_{j-}^2 + S_{i-}^2 S_{j+}^2) + V \sum_{\langle ij \rangle} S_{iz} S_{jz},$$

where $V > 0$, $t > 0$. The first single-site term in $\hat{H}$ describes the effects of a bare pseudo-spin splitting and relates with the on-site density-density interactions, or correlations: $\Delta = -U/2$. The second term, or a pseudospin Zeeman coupling may be related with a pseudo-magnetic field $\|Z$ which acts as a chemical potential $\mu$ for boson systems with a boson density constraint:

$$\frac{1}{N} \sum_i \langle S_{iz} \rangle = n,$$

where $n$ is the deviation from a half-filling ($n = 0$).

The third (Ising) term in $\hat{H}$ describes the effects of the short- and long-range inter-site density-density interactions. The last term in $\hat{H}$ describes the two-particle intersite hopping. In the strong on-site attraction limit of the model (large easy-axis pseudospin on-site anisotropy) we arrive at the Hamiltonian of the hard-core, or local, bosons which was earlier considered to be a starting point for explanation of the cuprate high-$T_c$ superconductivity [6]. The spin counterpart of $\hat{H}$ corresponds to an anisotropic $S = 1$ magnet with a single ion (on-site) and two-ion (bilinear and biquadratic) symmetric anisotropy in an external magnetic field. It describes an interplay of the Zeeman, single-ion and two-ion anisotropic terms giving rise to a competition of an (anti)ferromagnetic order along $Z$-axis with an in-plane $XY$ spin-nematic order. A remarkable feature of the Hamiltonian (1) is that the on-site pseudospin states $M = 0$ and $|M| = 1$ do not mix under the inter-site coupling. The model allows us to directly study a continuous transformation of the semi-hard-core bosons to the effective hard-core bosons formed by boson pairs under driving the correlation parameters $\Delta = -U/2$ to large negative values (“negative-$U$ model”). The simplified model can be directly applied to a description of bosonic systems with suppressed one-particle hopping.

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3. Mean-field approximation

To analyse the simplified model we start with a mean-field approximation (MFA) for 2D square lattice, however, at variance with a conventional classical MFA we made use of more correct approach that takes into account the quantum nature of the $S - 1$ (pseudo) spin states [7]. First we introduce a set of the on-site $S - 1$ coherent states

$$|\phi_i\rangle = c_i |\uparrow\rangle + c_{i+1} |\downarrow\rangle,$$

where the $c_M$ coefficients can be represented as follows

$$c_1 = \sin \frac{\theta}{2} \cos \phi \frac{e^{-i\frac{\phi}{2}}}, \quad c_0 = \cos \frac{\theta}{2} e^{i\frac{\phi}{2}},$$

$$c_{-1} = \sin \frac{\theta}{2} \sin \phi \frac{e^{i\frac{\phi}{2}}}$$

with $\theta, \phi, \alpha, \beta$ to be parameters defined by the minimization of the energy. The MFA energy can be written as follows

$$E = \frac{V}{2} \sum_i (1 - \cos \theta_i) - \frac{\mu}{2} \sum_i (1 - \cos \theta_i) \cos \phi_i$$

$$+ \frac{\nu}{4} \sum_{\langle ij \rangle} (1 - \cos \theta_i)(1 - \cos \theta_j) \cos \phi_i \cos \phi_j$$

$$- \frac{\Delta}{2} \sum_{\langle ij \rangle} (1 - \cos \theta_i)(1 - \cos \theta_j) \sin \phi_i \sin \phi_j \cos (\alpha_i - \alpha_j).$$

It is worth noting that due to the absence of the one-particle inter-site hopping terms in Hamiltonian (1) the energy does not depend on phase parameter $\beta$, so the $\beta$ remains undetermined. Below we denote $\delta = \Delta/t$ and $v = V/t$. In a two-sublattice A-B model we arrive at a high-temperature non-ordered (NO) phase and the five MFA uniform phases, two phases with nonzero local superfluid order parameter, or pseudospin nematic order $\langle S_{A,B}^2 \rangle \neq 0$ and three charge ordered phases with $\langle S_{A,B}^2 \rangle = 0$ but different types of the sublattice occupation (pseudospin $S_z$ components):

**Superfluid (SF) phase:** $\langle S_{A,B}^2 \rangle = n$, $\langle S_{A,B}^4 \rangle = 1$, $\langle S_{A,B}^2 \rangle = \frac{1}{2} \sqrt{1 - n^2 + 2 \zeta e^{\pm i\alpha}}$, uncertain factor $\zeta = \pm 1$.

**Supersolid (SS) phase:** $\langle S_{A,B}^2 \rangle = n$, $\langle S_{A,B}^4 \rangle = 1$, $\langle S_{A,B}^2 \rangle = \zeta e^{\pm i\alpha}$

$$\left(\sqrt{|n|} \sqrt{\frac{2n+1}{2n+1} - n^2} \pm \frac{\alpha}{\sqrt{2n+1} - n^2}\right).$$

Charge ordered COI phase: $\langle S_{A,B}^2 \rangle = 0$, $\langle S_{A,B}^4 \rangle = 0$, $\langle S_{B^2}^2 - 2n, S_{B^2}^2 - 2|n|, |n| \leq 0.5\rangle$.

Charge ordered COII phase: $\langle S_{A,B}^2 \rangle = 0$, $\langle S_{A,B}^4 \rangle = 0$, $\langle S_{B^2}^2 - 2n, S_{B^2}^2 - 2|n|, |n| \leq 0.5\rangle$.

Charge ordered COIII phase: $\langle S_{A,B}^2 \rangle = 0$, $\langle S_{A,B}^4 \rangle = 0$, $\langle S_{B^2}^2 - 2n, S_{B^2}^2 - 2|n|, |n| \leq 0.5\rangle$.

Interestingly, all the local order parameters do not depend on the correlation parameter $\Delta$, while this parameter governs the energy of different phases. Taking into account the on-site correlations we arrive at very rich and intricate phase diagrams for the model system as compared with relatively simple phase diagrams for hard-
core bosons [6, 8]. In Fig. 1 (dotted curves) we present an example of the MFA \( \delta - n \) phase diagrams calculated given \( v = 0.75 \). At half-filling \( n = 0 \) the positive values of the correlation parameter \( \delta \) stabilize a limiting COI phase with \( \langle S_{A,Bz} \rangle \neq \langle S_{A,Bz}^2 \rangle = 0 \), or a “parent \( \mathrm{Cu}^{2+} \) phase” for a model cuprate, while positive values of \( v \) stabilize a limiting COII phase with \( \langle S_{A,Bz} \rangle = \pm 1; \langle S_{A,Bz}^2 \rangle = 1 \), or a checkerboard “antiferromagnetic” order of pseudospins along \( z \)-axis, or a disproportionated \( \mathrm{Cu}^{1+} \)-\( \mathrm{Cu}^{3+} \) phase for a model cuprate. As a result of the competition between the on-site and inter-site correlations we arrive at a “starting” COI phase for \( \delta > 2v \) or COII phase for \( \delta \leq 2v \). At \( n = 0.5 \) we see a transformation of the COI and COII phases into the COIII phase. The line of the first order phase transition COIII-SF in Fig. 1 corresponds to the equality of the respective energies. It is worth to note that the critical concentration \( n \) for the SS-SF, COI, COII-COIII transitions does not depend on the correlation parameter \( \delta \). In Fig. 2 (top panel, solid lines) we present the \( n \)-dependence of the correlation functions \( S_{zz}(\pi,\pi) - \langle S_z, S_z \rangle \) (static structure factor) and \( S_{zz}^2(0,0) - \langle S_z^2, S_z^2 \rangle \) at \( \delta = 1.5, v = 0.75 \), determining the long-range CO and SF orders, respectively, given \( \Delta/t = 1.5 \), that is in an immediate closeness to COII-COI phase transition for small \( n \).

4. Quantum Monte-Carlo calculations

We have performed Quantum Monte-Carlo (QMC) [9] calculations for our model Hamiltonian (1). In Fig. 1 (solid lines) we compare the ground state \( \delta - n \) phase diagram of our model 2D system calculated on square lattice \( 8 \times 8 \) given \( v = 0.75 \) with that of calculated within MFA approach. As for simple hard-core counterpart [6,8], despite some qualitative agreement, we see rather large quantitative difference between two curves in Fig. 1. In particular, it concerns a clearly larger volume of the quantum SF phase that might be related with a sizeable suppression of quantum fluctuations within MFA approach. In Fig. 2 (top panel, two dotted lines) we present the QMC calculated static structure factor \( S_{zz}(\pi,\pi) \) and the superfluid (pseudospin nematic) correlation function \( S_{zz}(0,0) \). It is worth to note a semiquantitative agreement with the MFA data. Smaller value of the quantum structure factor \( S_{zz}(\pi,\pi) \) at \( n = 0 \) is believed to be a result of the pseudospin reduction due to quantum fluctuations. Bottom panel in Fig. 2 shows the \( n \)-dependence of the mean sublattice \( S_z \) values, \( S_{Az} \) and \( S_{Bz} \), that clearly demonstrates the pseudospin quantum reduction effect within COII phase and specific features of the sublattice occupation, or “pseudo-magnetization” under COII-COIII-SF transformation.

5. Conclusions

A simplified 2D \( S = 1 \) pseudospin Hamiltonian with a two-particle transport term (pseudospin nematic coupling) was analyzed within a generalized MFA and QMC technique.

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